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ANISOTROPIC RELAXATION FUNCTIONS AND STRENGTH
OF ORIENTED SOLIDS

S . R. Moghe and C. C. Hsiao
University of Minnesota, Minneapolis, Minnesota

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S. R. Moghe and C. C. Hsiao
University of Minnesota, Minneapolis, Minnesota

Mechanical properties of a solid are formulated in terms of microscopic behavior as a result of deformation and orientation. The relaxation behavior of the oriented solid is obtained by considering statistically the viscoelastic micro behaviors. It is found that various anisotropic relaxation functions can be expressed as a single time-dependent function under certain conditions. The time-dependent macroscopic fracture strength is also analyzed for the oriented system using known results for a completely oriented system.

Author

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INTRODUCTION

In this report a phenomenological theory of the time dependent characteristics of anisotropic relaxation functions as well as strength of oriented viscoelastic media is presented. In obtaining the relaxation functions viscoelastic behavior for microscopic components in the media has been considered. However, in formulating the conditions of the time-dependent fracture strength, viscous behavior was not taken into account as fracture is unlikely to occur when flow deformation exists. Thus the analysis applies to elastic medium, but the nature of molecular orientation effect resulted in from large flow deformation was included. Essentially, attempts are made to extend an earlier theory investigated during the last few years.¹⁻⁴ The basic mathematical model is a matrix of oriented linear elastic elements embedded in an arbitrary domain. The elements representing molecular forces constitute an ideal medium which has been found quite useful in predicting macrobehavior including ultimate strength under simple external loading conditions. Assuming the homogeneity of the medium, the macroscopic properties can be deduced through the analysis of the state of stress in a small neighborhood of a point attached with microscopic constituents represented by deformable vectors. In spherical coordinates (θ, ϕ) the stress tensor at a point may be expressed as follows:^{1,2:}

$$\sigma_{ij} = \int \rho(\theta, \phi, \epsilon) f(\theta, \phi, t) \psi(\theta, \phi) s_i s_j d\omega \quad (1)$$

where $\rho(\theta, \phi, \epsilon)$ is the density of probability distribution function of orientation associated with a state of strain ϵ , $f(\theta, \phi, t)$ is the fraction of elements that are available at

the time of consideration. $\psi(\theta, \phi)$ is the stress in the axial direction of an element in the matrix. s_i and s_j are unit vectors whose components in spherical coordinates are $(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ and $d\omega$ is the infinitesimal solid angle.

For small deformations the complete matrix will have little or no orientation effect. However, when deformations become appreciable, the orientation of microelements must be taken into consideration if significant result is to be obtained. This can be accomplished through the use of $\rho(\theta, \phi, \epsilon)$ in terms of a state of strain ϵ . Depending upon the nature of molecular constitution, two extreme cases or their combinations may be considered. For randomly oriented elements, if ϵ is a simple homogeneous large strain:¹

$$\rho(\theta, \phi, \epsilon) = \frac{(1+\epsilon)^3}{[\cos^2\theta + (1+\epsilon)^3 \sin^2\theta]^{3/2}} \rho(0) \quad (2)$$

where $\rho(0) = 1/4\pi$ is a constant representing a random distribution density function of orientation. In the case if the elements are connected by flexible joints, then:^{2*}

$$\rho(\theta, \phi, \epsilon) = \frac{\alpha}{[\cos^2\theta/2 + \alpha \sin^2\theta/2]^2} \rho(0) \quad (3)$$

where α is associated with ϵ as follows:

$$\epsilon = 1 + \frac{8\alpha}{\alpha^2 - 1} \ln \frac{\alpha + 1}{2\alpha} \quad (4)$$

The quantity $f(\theta, \phi, t)$ is derivable from the theory of absolute reaction rate as

$$\frac{df}{dt} = K_r(1 - f) - K_b f \quad (5)$$

*For additional references refer to 2.

where

$$K_r = \omega_r e^{-U/RT - \gamma\psi(\theta, \phi, t)}$$

and

$$K_b = \omega_b e^{-U/RT + \beta\psi(\theta, \phi, t)}$$

(6)

are respectively the rate coefficients for reformation and breakage of elements. ω_r , ω_b , γ , β , U and R are material constants and T is the absolute temperature.

MACROSCOPIC RELAXATION FUNCTIONS

In determining macroscopic relaxation functions, one way is to extend the formulation (1) through the consideration of the viscoelastic behavior of the individual micro-elements. If a one-dimensional constitutive equation of individual elements is considered, the stress in general is expressible as a functional of deformation history subject to the restrictions imposed upon by the principles of objectivity. Under suitable restrictions and for small finite deformations e , $\psi(t)$ can be expressed as

$$\begin{aligned} \psi(t) = & \int_0^t E(t - \tau) \dot{e}(\tau) d\tau \\ & + \int_0^t \int_0^t F(t - \tau_1, t - \tau_2) \dot{e}(\tau_1) \dot{e}(\tau_2) d\tau_1 d\tau_2 \\ & + \dots \end{aligned} \tag{7}$$

where the kernel functions E , F , etc. depend upon the microscopic relaxation behavior of the elements. If the deformation e is small, the first integral in (7) alone will be sufficient for a good representation of the viscoelastic behavior.

For a smooth function $e(t)$ it can be shown that $\psi(t)$ will also be a smooth function. Then an inspection of (5) in view of (7) will show that $f(t)$ is also a smooth function of time for a given initial value f_0 . Therefore, starting with a number of unbroken elements f_0 the traction force contribution by these elements at any time t will depend upon the entire history of $f(t)$ during the time interval $(0, t)$ in view of (5) and (7). This contribution will increase or decrease according to the number of unbroken elements increases or decreases. Any reformation or breakage of the elements in an interval $(0, \tau)$ smaller

than $(0, t)$ will affect the traction force contribution at time t . Then through the application of superposition principle we can modify (1) as

$$\sigma_{ij}(t) = \int_{\omega} \rho(\theta, \phi, \epsilon) s_i s_j \int_0^t f(\theta, \phi, t, \tau) d\psi(\theta, \phi, \tau) d\omega \quad (8)$$

Assuming $\psi(t)$ to be a differentiable function, we can write (8) as

$$\sigma_{ij}(t) = \int_{\omega} \int_0^t \rho(\theta, \phi, \epsilon) s_i s_j f(\theta, \phi, t, \tau) \frac{\partial \psi(\theta, \phi, \tau)}{\partial \tau} d\tau d\omega \quad (9)$$

provided the integrals exist. If we assume now that any reformation or breakage of elements in the past will influence, in a consistent manner, the traction force contribution or stress tensor at time t then (9) can further be modified as

$$\sigma_{ij}(t) = \int_{\omega} s_i s_j \int_0^t \rho(\theta, \phi, \epsilon) f(\theta, \phi, t - \tau) \frac{\partial \psi(\theta, \phi, \tau)}{\partial \tau} d\tau d\omega \quad (10)$$

Substituting for $\psi(t)$ from (7) into (10) we obtain

$$\begin{aligned} \sigma_{ij}(t) = & \int_{\omega} s_i s_j \rho(\theta, \phi, \epsilon) s_m s_n \\ & \cdot \int_0^t f(\theta, \phi, t - \tau) \frac{d}{d\tau} \int_0^{\tau} E(\tau - \lambda) \dot{e}_{mn}(\lambda) d\lambda d\tau d\omega \end{aligned} \quad (11)$$

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Simplifying further we get

$$\begin{aligned} \sigma_{ij}(t) = & \int_{\omega} \rho(\theta, \phi, \epsilon) s_i s_j s_m s_n \left[\int_0^t f(\theta, \phi, t - \tau) E(0) \dot{e}_{mn}(\tau) d\tau \right. \\ & \left. + \int_0^t f(\theta, \phi, t - \tau) \int_0^{\tau} \dot{E}(\tau - \lambda) \dot{e}_{mn}(\lambda) d\lambda d\tau \right] d\omega \end{aligned} \quad (12)$$

+

For simplicity, here, the higher order terms are not shown.

Through the use of Laplace transform it can be shown that for infinitesimal deformations,

$$\sigma_{ij}(t) = \int_0^t C_{ijmn}(t - \tau) \dot{e}_{mn}(\tau) d\tau \quad (13)$$

where

$$C_{ijmn}(t) = \int_{\omega} \rho(\theta, \phi, \varepsilon) s_i s_j s_m s_n \int_0^t f(\theta, \phi, t - \tau) \dot{E}(\tau) d\tau d\omega \quad (14)$$

which can be computed. Here $C_{ijmn}(t)$ is a symmetrical tensor defined as $C_{ijmn}(t) = C_{mni j}(t)$. Also, the comparison with the transversely isotropic elastic solid as reported earlier^{1,3} indicates that there are only three independent time dependent functions involved in (14). In general for a transversely isotropic solid, which can be resulted in from a uniaxial orientation, there are five independent functions $C_{ijmn}(t)$. The absence of two of these functions in the present case can be attributed to the limitation on the simple model for which the Cauchy relations are identically satisfied. A more general model may remove this limitation.

In order to determine $C_{ijmn}(t)$ from (14) it is necessary to solve (5) which by no means is an easy task. Only numerical method of solutions of (5) and (14) will produce some concrete results. However, in some cases as when f in (5) may be a slowly varying function, i.e. $f \simeq 0$ the evaluation of (14) is somewhat easier. Under a very restricted assumption that $f(\theta, \phi, t) = f(t)$, (14) takes a very simple form

$$C_{ijmn}(t) = \int_{\omega} \rho(\theta, \phi, \varepsilon) s_i s_j s_m s_n d\omega \int_0^t f(t - \tau) \dot{E}(\tau) d\tau \quad (15)$$

where only one time dependent function is involved. In this case, referring to a spherical coordinate system and locating the direction of any representative element by angles θ and ϕ the joint probability distribution function is

$$\int_0^\phi \int_0^\theta \frac{1}{2\pi} \sin\theta d\theta d\phi \quad \begin{array}{l} 0 \leq \theta \leq \pi/2 \\ 0 \leq \phi \leq 2\pi \end{array}$$

Finally if $\rho(\theta, \phi, \epsilon)$ is given as in (2) then

$$\begin{aligned} c_{1111}(t) &= c_{2222}(t) = \frac{3}{8}\rho(0)[1 - 2F_1 + F_2]G(t) \\ c_{1122}(t) &= \frac{1}{3}c_{1111}(t) = \frac{1}{8}\rho(0)[1 - 2F_1 + F_2]G(t) \\ c_{1133}(t) &= c_{2233}(t) = \frac{1}{2}\rho(0)[F_1 - F_2]G(t) \\ c_{3333}(t) &= \rho(0)F_2G(t) \end{aligned} \quad (16)$$

where $F_1 \equiv \frac{1}{k^2}[1 - (1 - k^2)^{\frac{1}{2}} \frac{\sin^{-1}k}{k}]$

$$F_2 \equiv 3 - k^2 - 3(1 - k^2)^{\frac{1}{2}} \frac{\sin^{-1}k}{k}$$

$$k^2 \equiv 1 - (1 + \epsilon)^{-3}$$

and

$$G(t) \equiv \int_0^t f(t - \tau) \dot{E}(\tau) d\tau$$

These results show that if $G(t)$ is determined experimentally by one type of test, then all the anisotropic functions are obtainable by multiplying with their corresponding coefficients. Fig. 1 shows the variation of these coefficients in $El^2\lambda f_0$ where l is length of the elements and λ the number of elements in a unit volume. It is interesting to observe that if a system like this exists, the anisotropic relaxation functions behave very much alike. This seems reasonable as a molecular system is essentially composed of similar molecular elements. Under load somewhat similar behavior may be expected.

TIME DEPENDENT MACRO-STRENGTH

Investigations concerned with the time dependent fracture of completely oriented solids under simple loading conditions have been reported.^{4,5} Analytical considerations for partially oriented systems under general loads are not yet available. The time dependent fracture of any medium can be studied by solving (5) and (12) together with a fracture criterion. Here we are looking for a relation between time-to-fracture t_b and applied stresses $\sigma_{ij}(t)$. In dealing with such a problem, the large flow deformation is considered to contribute to the molecular orientation only whereas the small elastic deformations will govern the fracture mechanism of the elements and thus the strength of the solid.

Under moderate and large loading conditions, consider (1) in the following modified form.

$$\sigma_{ij}(\epsilon, t) = \int_{\omega} \rho(\theta, \phi, \epsilon) f(\theta, \phi, t) \psi(\theta, \phi, t) s_i s_j d\omega \quad (17)$$

where, in the absence of reformation processes i.e. $K_r \equiv 0$, f satisfies

$$\frac{df}{dt} = -K_b f = -\Omega_b e^{\beta\psi} f \quad (18)$$

and

$$\Omega_b \equiv \omega_b e^{-U/RT}$$

For constant loading $\sigma_{ij} = \text{constant}$, differentiation of (17) with respect to t gives

$$0 = \int_{\omega} \rho(\theta, \phi, \epsilon) \left[f \frac{\partial \psi}{\partial t} + \psi \frac{\partial f}{\partial t} \right] s_i s_j d\omega \quad (19)$$

Multiply (18) by $\rho(\theta, \phi, \varepsilon) s_i s_j \psi(\theta, \phi, t)$ and integrate over the entire volume then

$$0 = \int_{\omega} \rho(\theta, \phi, \varepsilon) \psi(\theta, \phi, t) \left[\frac{df}{dt} + \Omega_b f e^{\beta \psi} \right] s_i s_j d\omega \quad (20)$$

where f is not zero at all times and for any s_i . Using (19) we can show that this equation is satisfied only if

$$\frac{\partial \psi}{\partial t} = \Omega_b \psi e^{\beta \psi} \quad (21)$$

This holds true for any arbitrary element defined by the spherical coordinates (θ, ϕ) . For a fully oriented medium if every element is oriented along 33-direction under a constant simple tension σ_{33} , then (21) can be expected to be true for the entire homogeneous solid as the strength behavior of the entire solid is representable by that of an individual element. Assuming that all the elements are identical and would break when $\psi(\theta, \phi, t) \rightarrow \psi_b$, then this will serve as an adequate criterion for obtaining the required time-dependent fracture information. Of course, other maximum strain criterion or maximum energy criteria may also be used. If we do not assume any of those, the natural criterion which results from the definition of f is that fracture will occur when $f \rightarrow 0$.

Now we consider that initially when $t = 0$, $f = 1$ and $\psi = \psi_0$ then integrating (21) we get

$$t_b = \frac{1}{\Omega_b} [Ei(-\beta \psi_b) - Ei(-\beta \psi_0)] \quad (22)$$

This is the equation giving the time-to-break for any individual element along the direction indicated by (θ, ϕ) for any ψ_0 at $t = 0$. $Ei(-x)$ is the exponential integral of argument x defined by

$$-Ei(-x) = \int_x^{\infty} \frac{e^{-y}}{y} dy \quad (23)$$

From the definition, $\psi_o(\theta, \phi) = Ee_{mn}s_ms_n$ at $t = 0$ then substituting into (17) we get

$$\sigma_{ij} = EC_{ijmn}e_{mn} \quad (24)$$

where

$$C_{ijmn} = \int_{\omega} \rho(\theta, \phi, \epsilon) s_i s_j s_m s_n d\omega \quad (25)$$

If we define B_{ijmn} as the inverse of C_{ijmn} such that

$$\|B_{ijmn}\| = \|C_{ijmn}\|^{-1} \quad (26)$$

then

$$Ee_{mn} = B_{ijmn}\sigma_{ij} = B_{ijmn}\sigma_{mn} \quad (27)$$

and finally

$$\psi_o(\theta, \phi) = B_{ijmn}\sigma_{ij}s_ms_n \quad (28)$$

Here both C_{ijmn} and B_{ijmn} are functions of orientation strain $\epsilon^{1,3}$. Then (22) can be expressed as

$$t_b = \frac{1}{\Omega_b} [Ei(-\beta\psi_b) - Ei(-\beta B_{ijmn}\sigma_{mn}s_is_j)] \quad (29)$$

which essentially gives $t_b = t_b(\sigma_{ij}, s_i)$. It is obvious from (29) that the elements oriented in different directions initially will break at different times, and the choice of the time-to-break for the entire solid becomes very difficult or arbitrary. However, a statistical average with respect to the distribution function $\rho(\theta, \phi, \epsilon)$ will hopefully give a more representative value to t_b . For a continuous distribution of elements, as in the present case, the average representative time-to-break \bar{t}_b may be given by

$$\bar{t}_b = \int_{\omega} t_b(\theta, \phi) \rho(\theta, \phi, \epsilon) d\omega / \int_{\omega} \rho(\theta, \phi, \epsilon) d\omega \quad (30)$$

If $\rho(\theta, \phi, \epsilon)$ as defined in (2) is considered, then (30) becomes

$$\bar{t}_b = \int_{\omega} \frac{(1 + \epsilon)^3}{[\cos^2 \theta + (1 + \epsilon)^3 \sin^2 \theta]^{3/2}} t_b(\theta, \phi) d\omega / 2\pi \quad (31)$$

Substitute (29) in (31), we obtain

$$\begin{aligned} \bar{t}_b = \frac{1}{\Omega_b} & \left[\text{Ei}(-\beta \psi_b) \right. \\ & \left. - \int_{\omega} \frac{\text{Ei}(-\beta B_{ijmn} \sigma_{ij} s_m s_n) (1 + \epsilon)^3}{[\cos^2 \theta + (1 + \epsilon)^3 \sin^2 \theta]^{3/2}} d\omega / 2\pi \right] \quad (32) \end{aligned}$$

For an isotropic solid $\epsilon = 0$, then

$$\bar{t}_b = \frac{1}{\Omega_b} [\text{Ei}(-\beta \psi_b) - \text{Ei}(-\beta B_{ijmn}(0) \sigma_{ij} s_m s_n)] \quad (33)$$

where $B_{ijmn}(0) = B_{ijmn}|_{\epsilon=0}$

Evaluation of the integral (33) will give the required result.

It may be emphasized that such explicit results cannot be obtained if the reformation processes are considered i.e. $K_r \neq 0$ in (5).

To obtain some intuition about the results in (32), let us consider a triaxial state of stress $\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma$ (say), and the medium isotropic, then it can be shown³ that $B_{ijmn} \sigma_{ij} s_m s_n = 3\sigma$. Substituting into (24) we obtain

$$\bar{t}_b = \frac{1}{\Omega_b} [\text{Ei}(-\beta \psi_b) - \text{Ei}(-3\beta \sigma)] \quad (34)$$

which has a behavior as shown in Fig. 2. This is

qualitatively similar to that given earlier⁴ when reformation processes are neglected. Equation (34) enforces a natural limitation on the maximum value σ_m of σ since \bar{t}_b cannot be negative. This value σ_m is given by setting $\bar{t}_b = 0$ in (34) to be $\psi_b/3$. Similar results can also be obtained when different possible loadings and orientations are considered.

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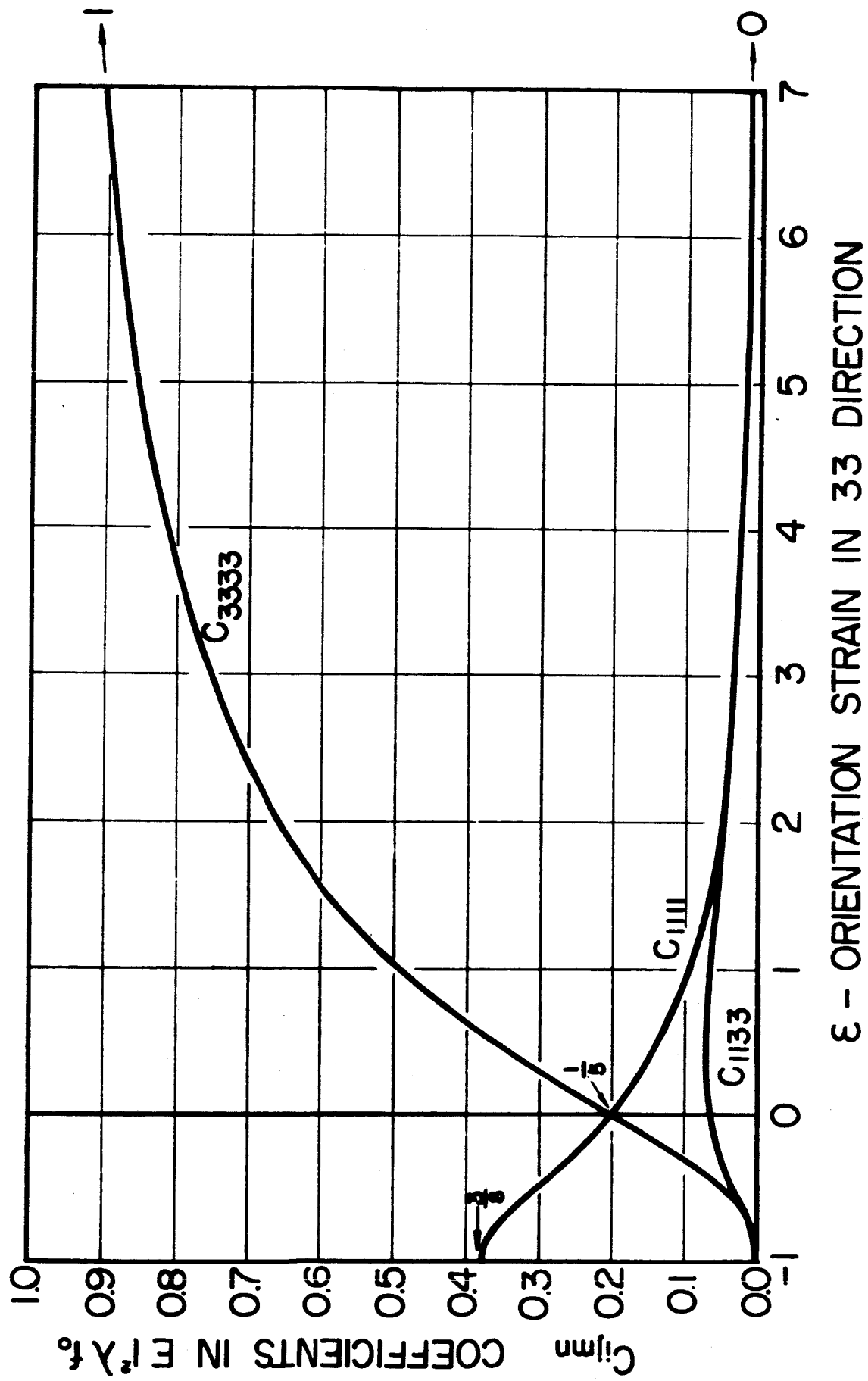


Fig. 1 Variations of Relaxation Coefficients

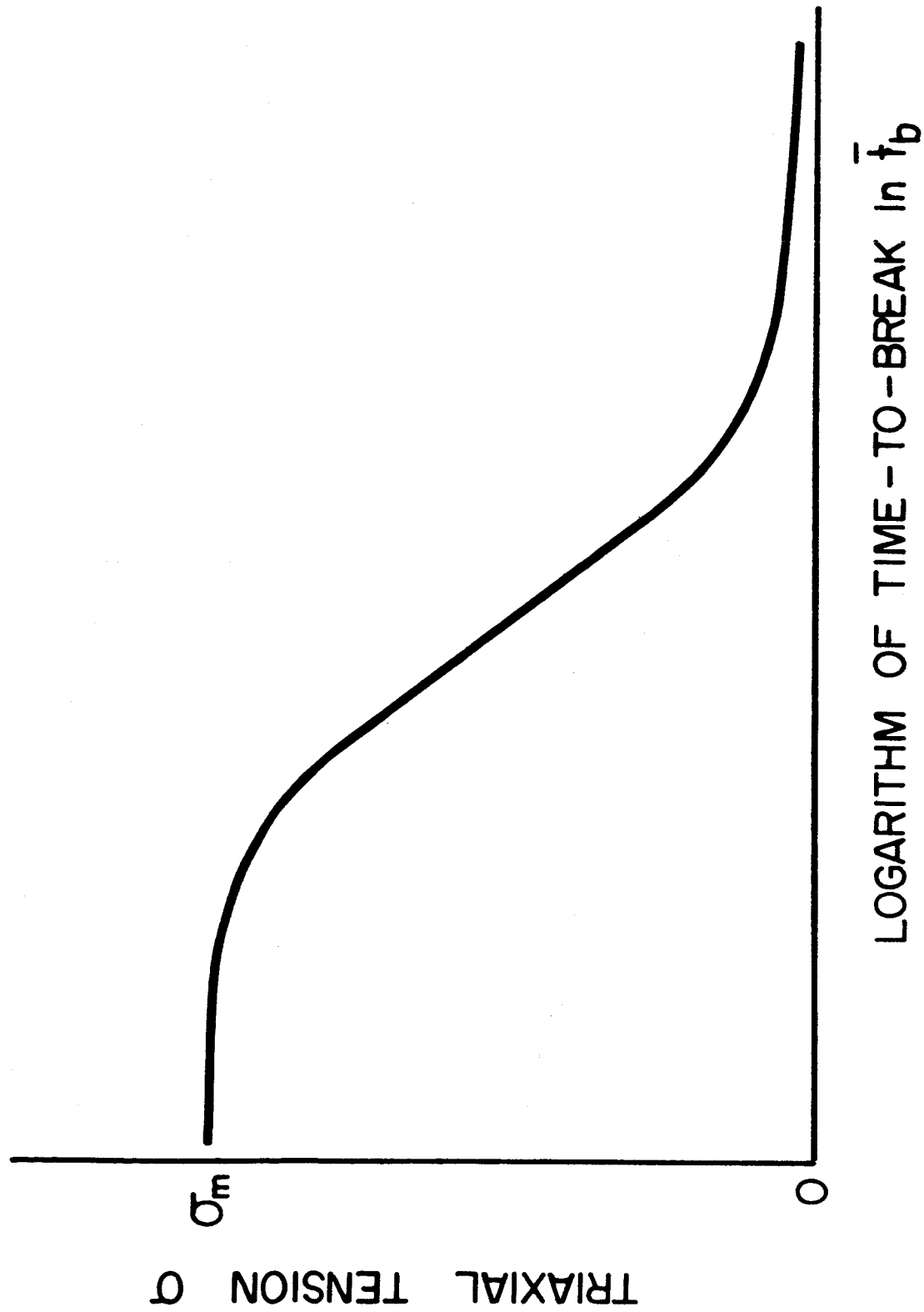


Fig. 2 Time-Dependent Strength under Triaxial Tension